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## Centre for Advanced Materials for Integrated Energy Systems (CAM-IES)

### Kick Off meeting – January 2017 <u>WP4 Organic-inorganic hybrid interfaces -</u> <u>Spin triplet excitons for photovoltaics.</u>

WP4 Leader: Hugo Bronstein - UCL

#### Members

#### UCL

#### CAM

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Bronstein – WP Leader, Synthesis Cacialli – Devices, photophysics Clarke - Spectroscopy Papakonstantinou - Characterization Friend – Spectroscopy, Devices Greenham – Spectroscopy, Nanocrystals Rao – Spectroscopy, Devices

#### QMUL

Nielsen - Synthesis Gillin – Characterization, Spin

#### NCU

Gibson – Photo/electro chemistry Penfold – Simulation, Theory Cucinotta – Supramolecular chemistry





AIM: Increase the efficiency of inorganic PV through the use of Singlet Fission





1. Light Absorption





#### 2. Singlet Formation





3. Singlet Fission





















5. Triplet Injection





6. Photocurrent Generation



#### 1+2+3. Light Absorption/Singlet Fission

#### Singlet Fission has very strict energetic requirements



Brian J. Walker, Andrew J. Musser, David Beljonne, Richard H. Friend, Nature Chemistry 5, 1019–1024 (2013)

Linear acenes (tetracene, pentacene) almost exclusively used Suffer from poor stability and lack of tunability (limits choice of inorganic component)

#### TASK: Develop stable, tunable materials for singlet fission (UCL-CAM)



### **4. Triplet Diffusion**

Triplet diffusion in organic materials is not well understood. Large range of values ranging from ~ 0 (immobile) to 2 microns.



Triplet exciton diffusion in pentacene (a singlet fission material) found to be 40 nm.

Maxim Tabachnyk, Bruno Ehrler, Sam Bayliss, Richard H. Friend, and Neil C. Greenham, Applied Physics Letters 2013 103:15

TASK: Develop understanding of triplet diffusion in organic materials (i.e diffusion anisotropy, effect of morphology, exciton confinement etc..) (UCL)



### **5. Triplet Injection**

Direct injection of triplet excitons into an inorganic semiconductor has only recently been demonstrated from pentacene to PbSe



Efficient transfer seems to require resonance  $(\pm 0.2 \text{ eV})$  of the triplet energy with the bandgap of the inorganic semiconductor.

Effect of molecular orientation, distance, interlayers and energetics almost completely unexplored

Maxim Tabachnyk, Bruno Ehrler, Simon Gélinas, Marcus L. Böhm, Brian J. Walker, Kevin P. Musselman, Neil C. Greenham, Richard H. Friend, Akshay Rao, Nature Materials 13, 1033–1038 (2014)

TASK: Develop an understanding the nature of the interface between organic and inorganic semiconductors with an aim to increasing triplet injection (CAM)



### 6. Choice of Inorganic Semiconductor/Photocurrent Generation



Perovskite solar cells are of comparable efficiency to Silicon PV, and there are numerous other potential inorganic materials (eg ZnO, PbSe etc..). Each have their benefits and drawbacks.

Important to understand the generality of the inorganic-organic interface with different semiconductors. Also, possibility of chemical modification of some of these to directly link organic-inorganic components

TASK: Determine optimum inorganic materials for interface. Explore the possibility of surface modifications/functionalisation. (CAM)



#### **Looking Forward to It!**